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Special issue: Selected Papers from the 6th International
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Guest Editors: Shigeki Takishima, Yoshio Iwai and Theo de Loos

FLUID PHASE

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FLUID PHASE

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Fluid Phase Equilibria

Volume 357, Pages 1-86 (15 November 2013)

Selected Papers from the 6th International Symposium on Molecular Thermodynamics and Molecular Simulation, September 25-28, 2012, Hiroshima, Japan

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Application of Gibbs energy model to equilibrium potential for structural phase transition in lithium intercalation process

Original Research Article

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Eiji Tatsukawa, Tomohide Ikeda, Kazuhiro Tamura

Highlights

► Modeling of equilibrium potential of LiCoO_2 and LiFePO_4 . ► Activity correction for the Nernst equation of lithium intercalation reaction. ► Gibbs energy model for heterogeneous system. ► NRTL and Redlich-Kister equation are applied for the activity correction. ► Accurate simulation of equilibrium potential prediction is demonstrated.

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Liquid–liquid equilibria containing fluorosolvants as

environmentally benign solvent

Original Research Article

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Hiroyuki Matsuda, Yuki Hirota, Kiyofumi Kurihara, Katsumi Tochigi, Kenji Ochi

Highlights

► This study investigates measurements of LLE data containing two fluoruous solvents. ► Perfluorohexane and Galden® HT-135 were investigated as fluoruous solvent. ► LLE data of mixtures perfluorohexane + *n*-alkane (C⁷, C⁹, and C¹⁰) were measured. ► LLE data of mixtures Galden HT-135® + dibutyl ether / butyl acetate were also measured. ► Experimental LLE data were represented by NRTL model.

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